

Modeling soil heating and moisture transport under extreme conditions: Forest fires and slash pile burns

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[1] Heating any soil during a sufficiently intense wildfire or prescribed burn can alter it irreversibly, causing many significant, long-term biological, chemical, and hydrological effects. Given the climate-change-driven increasing probability of wildfires and the increasing use of prescribed burns by land managers, it is important to better understand the dynamics of the coupled heat and moisture transport in soil during these extreme heating events. Furthermore, improved understanding and modeling of heat and mass transport during extreme conditions should provide insights into the associated transport mechanisms under more normal conditions. The present study describes a numerical model developed to simulate soil heat and moisture transport during fires where the surface heating often ranges between 10,000 and 100,000 W m⁻² for several minutes to several hours. Basically, the model extends methods commonly used to model coupled heat flow and moisture evaporation at ambient conditions into regions of extreme dryness and heat. But it also incorporates some infrequently used formulations for temperature dependencies of the soil specific heat, thermal conductivity, and the water retention curve, as well as advective effects due to the large changes in volume that occur when liquid water is rapidly volatilized. Model performance is tested against laboratory measurements of soil temperature and moisture changes at several depths during controlled heating events. Qualitatively, the model agrees with the laboratory observations, namely, it simulates an increase in soil moisture ahead of the drying front (due to the condensation of evaporated soil water at the front) and a hiatus in the soil temperature rise during the strongly evaporative stage of the soil drying. Nevertheless, it is shown that the model is incapable of producing a physically realistic solution because it does not (and, in fact, cannot) represent the relationship between soil water potential and soil moisture at extremely low soil moisture contents (i.e., residual or bound water: $\theta < 0.01 \text{ m}^3 \text{ m}^{-3}$, for example). Diagnosing the model's performance yields important insights into how to make progress on modeling soil evaporation and heating under conditions of high temperatures and very low soil moisture content.

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1. Introduction

[2] Most studies of the coupled heat and moisture transport in soils have concentrated primarily on conditions that encompass “normal” ambient environmental conditions, i.e., those involving daily and seasonal variations in radiation, temperature, precipitation, etc. [e.g., Philip and De Vries, 1957; Milly, 1982; Novak, 2010; Smits et al., 2011]. But, a few studies have examined these processes under

more extreme conditions, i.e., those occurring during wildfires and prescribed burns [e.g., Aston and Gill, 1976; Campbell et al., 1995; Durany et al., 2010]. Although the physical principles and the basic equations of all these models are more or less the same, the emphasis of the different modeling regimes (i.e., normal versus extreme conditions) is different. Models developed for the former tend to focus on the movement of soil moisture and evaporation; whereas models developed to describe the latter emphasize soil temperatures and the duration of the soil heating.

[3] Amount and duration of soil heating, which in a modeling context are provided by the upper boundary condition, determine the depth of heat penetration. Associated with this depth are certain critical temperature thresholds. For example, soil temperatures in the range of 60–80°C for short periods of time are lethal to plant seeds, plant roots, and plant tissue in general and at temperatures approaching 120–160°C range microbial life is extinguished [e.g., Levitt, 1980;

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Jiménez Esquilín *et al.*, 2007; Choczynska and Johnson, 2009]. At higher temperatures often irreversible physical, chemical, mineral, and hydrologic changes begin to occur to the soil [e.g., DeBano *et al.*, 1998; Neary *et al.*, 2005; Cerdà and Robichaud, 2009; Massman *et al.*, 2010].

[4] As a consequence of this historical emphasis on soil heating and temperatures during fires, there have been many modeling studies that have focused solely on soil temperatures and the associated heat flow during these extreme events [e.g., Pafford *et al.*, 1985; Chinanzvanana *et al.*, 1986; Steward *et al.*, 1990; Oliveria *et al.*, 1997; Preisler *et al.*, 2000; Antilén *et al.*, 2006]. But modeling heat and moisture transport simultaneously is a much more difficult task and although such models [i.e., Aston and Gill, 1976; Campbell *et al.*, 1995; Durany *et al.*, 2010] have had some success at modeling soil temperatures during severe heating events, they have yielded somewhat disappointing simulations of the coupled soil moisture dynamics. For example, Albini *et al.* [1996] review the models of Aston and Gill [1976] and Campbell *et al.* [1995] and found that the earlier model was prone to instabilities and that the later model did not provide a fully faithful simulation of soil moisture content; similar conclusions were reached by Campbell *et al.* [1995] themselves. Likewise, the model of Durany *et al.* [2010] provides reasonable model performance when simulating soil temperatures, but the model “retained” soil volumetric moisture contents as high as 0.15 despite heating the soils to over 500 C. The present study attempts to diagnose these systemic failures at modeling coupled heat and moisture transport during the extreme heating events that occur during fires through the development and evaluation of the performance of a new numerical model for simulating coupled heat and moisture transport during fires.

2. Physical Processes and Model Equations

[5] The present model is a one-dimensional model that uses some of the same parameterizations and employs some of the same basic assumptions as Campbell *et al.* [1995]; but it also differs from this older model in many important aspects as well. One key similarity between these two models is that neither explicitly allows for the vertical movement of water during a soil heating event. This seems reasonable for the laboratory studies used to evaluate both the older model and present model because they employed cylindrical containers with solid bottoms, which preclude the possibility of a draining soil column. Nonetheless, future research (models) should examine whether the extreme gradients in moisture potential created during a fire might be sufficient to cause capillary water rise toward the soil drying front. As with the older model, the present model also includes advective (mass flow) effects associated with the rapid volatilization (and associated gas expansion) of the soil moisture during the heating events. On the other hand, the present model does not include any induced advective currents that may be caused by external temperature or pressure (nonvolatilization) effects. But this is not to say that such advective effects are not important or significant. In fact, they can completely overwhelm the normal diffusive mass fluxes exiting of the soil by directly injecting large quantities of combustion products into the soil [Massman *et al.*, 2010].

But as these in situ field observations of Massman *et al.* [2010] show, such effects are likely to be two-dimensional in nature (at least for a slash pile burn) and are likely to be driven by complex effects associated with the radiation and convection associated with the fire itself. Consequently these issues are not addressed with the present study because they are beyond its scope. (Note that the one-dimensional model of Durany *et al.* [2010] includes both vertical water movement and implicitly includes any possible one-dimensional (nonvolatilization) advective effects as well.)

[6] There are several ways the present model differs from that of Campbell *et al.* [1995]. First, the present model assumes that the soil volumetric specific heat is temperature dependent. Second, it also uses a different soil water retention curve, which better describes the moist end of the water retention curve than did the older model. Third, the present model also uses a different formulation for soil surface evaporative flux and also employs extrapolative lower boundary conditions rather than specifying them directly from observations. All these changes are intended to make the present model more physically realistic and easier to use for application to real fires.

2.1. Mass Conservation For Soil Moisture

[7] The total volumetric water content of a porous medium is $\rho_w\theta + \rho_v(\eta - \theta)$; where ρ_w (10^3 kg m^{-3}) is the density of water, ρ_v (kg m^{-3}) is the water vapor density, θ ($\text{m}^3 \text{ m}^{-3}$) is volumetric soil moisture, η ($\text{m}^3 \text{ m}^{-3}$) is the total porosity of the soil, and $(\eta - \theta)$ is the air filled porosity.

[8] After adjusting for advection and excluding soil hydraulic conductivity, Milly's [1982] results yield the following one-dimensional equation of mass conservation for water (liquid plus vapor):

$$\begin{aligned} \frac{\partial}{\partial t} [\rho_w\theta + \rho_v(\eta - \theta)] &= (\rho_w - \rho_v) \frac{\partial \theta}{\partial t} + \eta \frac{\partial \rho_v}{\partial t} \\ &= \frac{\partial}{\partial z} \left[D_{ve} \frac{\partial \rho_v}{\partial z} - (\eta - \theta) u_{vl} \rho_v \right] \end{aligned} \quad (1)$$

where t (s) is time, z (m) is soil depth (positive downward), D_{ve} ($\text{m}^2 \text{ s}^{-1}$) is the (equivalent) molecular diffusivity associated with the diffusive transport of water vapor in the soil's air-filled pore space, and u_{vl} (m s^{-1}) is the advective velocity associated with volatilization, which is discussed in more detail in section 2.5. D_{ve} is expressed as

$$D_{ve} = \frac{\tau(\eta - \theta)\mathcal{E}D_v}{1 - e_v/P_a}$$

where τ (m m^{-1}) is the tortuosity of soil, $\mathcal{E}$ (dimensionless) is the vapor flow enhancement factor, e_v (Pa) is the soil vapor pressure, and P_a (Pa) is the ambient pressure, D_v ($\text{m}^2 \text{ s}^{-1}$) is the molecular diffusivity of water vapor in air, and the $1 - e_v/P_a$ term in the denominator is the Stefan correction, also termed the mass flow factor. (Note that for modeling purposes the Stefan term is limited to a maximum value of 10/3 (i.e., $1/(1 - e_v/P_a) \leq 10/3$). This is similar to Campbell *et al.* [1995] and is required to minimize numerical problems caused by e_v becoming large with increasing temperatures, which will be detailed below.)

[9] In turn, D_v is a function of temperature and pressure:

$$D_v = D_{vST} \left(\frac{P_{ST}}{P_a} \right) \left(\frac{T_K}{T_{ST}} \right)^\alpha$$

where $D_{vST} = 2.12 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$, $P_{ST} = 101,325 \text{ Pa}$ is the standard pressure, T_K (K) is the soil temperature, $T_{ST} = 273.15 \text{ K}$ is the standard temperature, and the exponent $\alpha = 1.75$. There are several possible models for τ , three of which are $\tau = 0.66$ [Penman, 1940a, 1940b], $(\eta - \theta)\tau = 1 - [1 - (\eta - \theta)]^{2/3}$ [Du Plessis and Masliyah 1991], and $\tau = 0.66[(\eta - \theta)/\eta]^3$ [Moldrup et al., 1997]. The present study uses the model of Du Plessis and Masliyah [1991]. The parameterization of the enhancement factor is taken directly from Campbell et al. [1995]: $\mathcal{E} = (1 + 2f_w)k_a$, where the parameters f_w and k_a (discussed in section 2.4, which follows) are taken from the soil thermal conductivity model of Campbell et al. [1994]. But because $\rho_w \gg \rho_v$ the term $(\rho_w - \rho_v) \frac{\partial \theta}{\partial t}$ in equation (1) can be approximated by $\rho_w \frac{\partial \theta}{\partial t}$. Furthermore, $\rho_w \frac{\partial \theta}{\partial t} \gg \eta \frac{\partial \rho_v}{\partial t}$ can also be expected. Therefore, the conservation of mass for soil moisture for a nondraining soil, equation (1), can be reasonably approximated as follows:

$$\rho_w \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[D_{ve} \frac{\partial \rho_v}{\partial z} - (\eta - \theta) u_{vl} \rho_v \right] \quad (2)$$

2.2. The Kelvin Equation and Saturation Vapor Density

[10] The Kelvin equation is used to model the relative humidity in the soil pore space, h_s , as follows:

$$h_s = \exp [(M_w \psi) / (RT_K)] \quad (3)$$

where ψ (J kg^{-1}) is the soil moisture potential, $M_w = 0.018 \text{ kg mol}^{-1}$ is the molecular mass of water vapor, and $R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}$ is the universal gas constant. This last relation is important in order to relate the soil moisture variables, ρ_v and e_v to ψ . This is given next.

$$e_v = h_s e_{sat} = \{ \exp [M_w \psi / (RT_K)] \} e_{sat}(T_K) \quad (4)$$

where $e_{sat} = e_{sat}(T_K)$ (Pa) is the saturation vapor pressure, which is a function of T_K . Following Campbell et al. [1995], the present study also uses Richards' [1971] formulation for e_{sat} , i.e.,

$$e_{sat}(T_K) = P_{ST} \exp(13.3016\vartheta - 2.042\vartheta^2 + 0.26\vartheta^3 + 2.69\vartheta^4) \quad (5)$$

where ϑ (dimensionless) is the reduced temperature, $\vartheta = 1 - T_b/T_K$, and $T_b = 373.15 \text{ K}$. Although Richards Equation was originally developed for temperatures between -50 C and 140 C , it nevertheless is accurate up to the critical temperature of water, $T_{crit} = 373.95 \text{ C}$ (or 647.096 K). Assuming that water vapor is an ideal gas, then it follows that the saturation vapor density, ρ_{sat} (kg m^{-3}), is given as $\rho_{sat}(T_K) = e_{sat}(T_K)M_w/(RT_K)$.

[11] It is important to recognize that equation (5) should be restricted to temperatures, not only below the critical temperature, T_{crit} , but to all temperatures below that temperature, T_K^* , at which the saturation vapor pressure becomes comparable to the ambient pressure; i.e., $e_{sat}(T_K^*) = P_a$. For applications near one earth's atmosphere this yields: $T_K^* \leq 375 \text{ K}$. For the present study because $P_a = 92,000 \text{ Pa}$ at the location of the laboratory where the fire heating experiments were performed $T_K^* = 370.44 \text{ K}$. Unfortunately this lower temperature limit cannot be imposed on the present model without producing either an instability or a loss of convergence. The reason for this (and possible solutions to it and other model performance issues) can only be discussed in the context of other more fundamental model limitations and only after displaying and diagnosing the mathematical solution produced by the model. Therefore, for the time being the only limit imposed on equation (5) and $\rho_{sat}(T_K)$ will be that $e_{sat}(T_K) = e_{sat}(T_{crit})$ and $\rho_{sat}(T_K) = \rho_{sat}(T_{crit})$ whenever $T_K \geq T_{crit}$.

2.3. Model Water Retention Curve

[12] Mathematically, the water retention curve (WRC) is denoted most generally as $\theta = \theta(\psi, T_K)$, i.e., soil moisture is a function of both moisture potential and temperature. Historically most of the functions developed to describe WRCs have focused solely on $\theta = \theta(\psi)$ and there have been a variety of functions developed over the past several decades for specifying this simpler relationship [e.g., Fredlund and Xing, 1994]. The model of $\theta = \theta(\psi)$ used by Campbell et al. [1995] is the following one-parameter water retention curve originally developed by Campbell et al. [1993].

$$\theta(\psi) = \theta_l \left[1 - \frac{\ln(\psi/\psi_l)}{\ln(\psi_{od}/\psi_l)} \right] = -\frac{\theta_l}{\alpha_l} \ln \left(\frac{\psi}{\psi_{od}} \right) \quad (6)$$

where $\psi_{od} = -1 \text{ MJ kg}^{-1}$ is the water potential for oven dry soil, θ_l is the extrapolated value of the water content when $\psi = \psi_l = -1 \text{ J kg}^{-1}$, and $\alpha_l = \ln(\psi_{od}/\psi_l) = 6\ln(10)$. Although equation (6) may be adequate at the dry end of the water retention curve [Resurreccion et al., 2011], it is not necessarily adequate at the moist end [Campbell and Shiozawa, 1992].

[13] The present study uses the following relation, adapted from Campbell and Shiozawa [1992] and further augmented from the original by a temperature function ψ_T , to model the water retention curve as a function of both temperature and moisture potential:

$$\theta(\psi, T_K) = -\frac{\theta_l}{\alpha_l} \ln \left(\frac{\psi}{\psi_{od}} \psi_T \right) + \theta_h \left[1 + \left(\alpha_h \frac{\psi}{\psi_{od}} \psi_T \right)^4 \right]^{-\frac{1}{m}} \quad (7)$$

where θ_h ($\text{m}^3 \text{ m}^{-3}$), α_h (dimensionless), and m (dimensionless) are parameters obtained from Campbell and Shiozawa [1992]. The specific relationship between the parameters θ_h and α_h of the present model and the equivalent parameters A and α of Campbell and Shiozawa [1992] are (1) $\theta_h = A\rho_b/\rho_w$, where ρ_b (kg m^{-3}) is the bulk density of dry soil, and (2) $\alpha_h = \alpha\psi_{od}/g$, where g (9.81 m s^{-2}) is the acceleration due to gravity. It should also be mentioned that the soil moisture variable coded into the model itself is not

actually ψ , but rather ψ/ψ_{od} , which is mentioned here solely to explain the use of this ratio in equation (7).

[14] In this last equation ψ_T (dimensionless) results from the surface tension of water being temperature dependent [e.g., *Vargaftik et al.*, 1983; *Kestin et al.*, 1984] and for the present modeling purposes ψ_T is in essence the temperature function of *Salager et al.* [2010], which is given as

$$\psi_T = \frac{\beta_T + T_{ref}}{\beta_T + T_K} > 0 \quad (8)$$

where β_T (K) is a soil (or porous media) dependent parameter, which may range approximately between -500 K and -350 K [*Bachmann and van der Ploeg*, 2002] and T_{ref} (K) is a reference temperature, assumed here to always be approximately 293.15 K = 20 C. For the present purposes $\beta_T = -360$ K and because the initial soil temperatures during the laboratory studies of soil heating are always near 293.15 K, T_{ref} is always assigned the same value as the initial soil temperature. One important requirement of ψ_T (or any other comparable function) is that it must (and in the present case does) ensure that $\partial\theta/\partial T < 0$ in accordance with observations [e.g., *Olivella and Gens*, 2000; *Salager et al.*, 2010]. Because $\psi_T > 0$ needs to be fulfilled for all soil temperatures, this last requirement on $\partial\theta/\partial T$ means that for any soil temperature T_K , which is greater than some cutoff temperature, T_{cut} (where $T_{cut} < |\beta_T|$), then $\psi_T(T_K \geq T_{cut}) = \psi_T(T_{cut})$. For the present model T_{cut} is defined as that temperature such that $\psi_T(T_{cut}) = 4$. In other words, to avoid possible numerical problems $\psi_T \leq 4$ is required during all model simulations.

2.4. Conservation of Energy and Heat Flow

[15] Including the evaporation of soil moisture in the soil heat flow equation yields the following conservation of energy for the coupled soil heating and evaporation model:

$$C_s \frac{\partial T}{\partial t} - L_v \rho_w \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[\lambda_s \frac{\partial T}{\partial z} \right] - (\eta - \theta) \rho_a c_{pa} u_{vl} \frac{\partial T}{\partial z} \quad (9)$$

where T (C) is soil temperature; $C_s = C_s(\theta, T)$ ($\text{J m}^{-3} \text{K}^{-1}$) is the volumetric heat capacity of soil, which is a function of both soil temperature and soil moisture; $L_v = L_v(T, \psi) = (45,144 - 48T - M_w \psi)/M_w$ (J kg^{-1}) is the latent heat of vaporization (which is taken from *Campbell et al.* [1995]); $\lambda_s = \lambda_s(\theta, T)$ ($\text{W m}^{-1} \text{K}^{-1}$) is the thermal conductivity of the soil, which is also a function of both soil temperature and soil moisture; ρ_a (kg m^{-3}) is the mass density of the soil air, also a function of temperature; and c_{pa} ($\text{J kg}^{-1} \text{K}^{-1}$) is specific heat capacity of ambient air, which is a function of both temperature and the vapor density. But for the present purposes $c_{pa} \equiv 1010 \text{ J kg}^{-1} \text{K}^{-1}$ is a reasonable assumption.

[16] The model of soil thermal conductivity, λ_s , is taken directly from *Campbell et al.* [1994] and is summarized as follows (by using functional notation, $\lambda_s = \lambda_s(\theta, T)$, to specify the specific dependencies of the model variables on temperature and soil moisture).

$$\lambda_s(\theta, T) = \frac{k_w \theta \lambda_w(T) + k_a (\eta - \theta) \lambda_a(\theta, T) + k_m (1 - \eta) \lambda_m}{k_w \theta + k_a (\eta - \theta) + k_m (1 - \eta)} \quad (10)$$

where $\lambda_w(T)$ is the thermal conductivity of water; $\lambda_a(\theta, T) = \lambda_d(T) + \lambda_v(\theta, T)$ is the apparent thermal conductivity of air and is the sum of the thermal conductivity of dry air, λ_d , and water vapor, λ_v , which incorporates the effects of latent heat transfer; λ_m is the thermal conductivity of the mineral component of the soil, which is assumed to be independent of temperature and soil moisture; and k_w , k_a , and k_m (dimensionless) are generalized formulations of the de Vries weighting factors [*de Vries*, 1963]. In general, *Campbell et al.* [1994] formulate λ_v as a function of the latent heat of vaporization, the vapor diffusivity, D_v , the Stefan factor, the slope of the saturation vapor pressure, and the parameter $f_w(\theta, T)$ (mentioned earlier in regards to the evaporation enhancement factor and to be discussed shortly).

[17] The de Vries weighting factors all have the same general form, which is

$$k_* = k_*(\theta, T) = \frac{1}{3} \left[\frac{2}{1 + \left(\frac{\lambda_*}{\lambda_f} - 1 \right) g_a} + \frac{1}{1 + \left(\frac{\lambda_*}{\lambda_f} - 1 \right) (1 - 2g_a)} \right]$$

where the subscript asterisk refers to water, air, or mineral, in accordance with notation of equation (10), and g_a is the *de Vries* [1963] shape factor, an empirically determined model parameter, for which, in general, $g_a \approx 0.1$ [*Campbell et al.*, 1994; G. S. Campbell, personal communication, 2011]. $\lambda_f = \lambda_f(\theta, T)$ is a weighted mixture of the thermal conductivities of air and water, which is given as

$$\lambda_f(\theta, T) = \lambda_a(\theta, T) + f_w(\theta, T) [\lambda_w(T) - \lambda_a(\theta, T)]$$

$$f_w(\theta, T) = \frac{1}{1 + \left(\frac{\theta}{\theta_w} \right)^{q_w(T)}}$$

where θ_w is a soil-specific empirically determined model parameter, $q_w(T)$ is a soil-specific empirically determined model function, and $0 \leq f_w \leq 1$ depending on the degree of soil wetness: $f_w = 0$ for a dry soil and $f_w = 1$ for a wet soil. Numerical values for these model constructs are likewise obtained from *Campbell et al.* [1994] and *Campbell* (personal communication, 2011).

[18] The model for C_s is

$$C_s(\theta, T) = c_s(T) \rho_b + C_w(T) \theta \quad (11)$$

where $c_s(T) = c_{s0} + c_{s1}T$ ($\text{J kg}^{-1} \text{K}^{-1}$) is the specific heat capacity of soil; $C_w(T) = C_{w0} + C_{w1}T + C_{w2}T^2$ ($\text{J m}^{-3} \text{K}^{-1}$) is the volumetric heat capacity of water; and c_{s0} , c_{s1} , C_{w0} , C_{w1} , and C_{w2} are model constants, of which four (c_{s0} , C_{w0} , C_{w1} , and C_{w2}) are relatively easy to specify and are given next: $c_{s0} = 0.87 \times 10^3 \text{ J kg}^{-1} \text{K}^{-1}$ [after *Campbell et al.*, 1995], $C_{w0} = 4.216 \times 10^6 \text{ J m}^{-3} \text{K}^{-1}$, $C_{w1} = -0.16 \times 10^4 \text{ J m}^{-3} \text{K}^{-2}$, and $C_{w2} = 0.17 \times 10^2 \text{ J m}^{-3} \text{K}^{-3}$. But c_{s1} ($\text{J kg}^{-1} \text{K}^{-2}$) has not been measured for many soils. The data and analysis of *Kay and Goit* [1975] suggest that $c_s(T)$ increases linearly with temperature with a slope, c_{s1} , ranging between $2.0 \text{ J kg}^{-1} \text{K}^{-2}$ and $3.5 \text{ J kg}^{-1} \text{K}^{-2}$. But these data are valid only between -73 C and 27 C, so it would seem worthwhile to examine

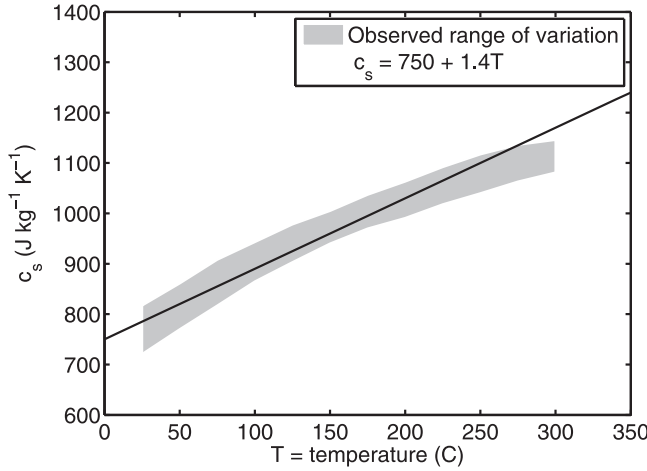


Figure 1. Heat capacity of a dry soil as a function of temperature. Shaded area shows range of variation of laboratory observations from soil samples obtained at Manitou Experimental Forest in the central Rocky Mountains of Colorado (see *Massman et al.* [2008] for further details). Solid line is a subjective estimate of the observed temperature dependency, where the relevant parameter for modeling studies is the slope.

$c_s(T)$ at soil temperatures that occur during fires. Figure 1 presents such data and shows the variation in heat capacity of a dry soil as a function of temperature in the range 25 °C to 300 °C. These data were obtained in the laboratory as part of a larger study of the long-term impact of soil heating on soils at the Manitou Experimental Forest (central Colorado, USA) [*Massman et al.*, 2008, 2010]. These data suggest that $c_s(T)$ may not increase linearly with increasing temperature. Nonetheless, approximating these data by a linear function yields a value of $c_{s1} \approx 1.4 \text{ J kg}^{-1} \text{ K}^{-2}$, which is somewhat less than found by *Kay and Goit* [1975]. For the present study neither the exact functional dependency (linear versus nonlinear) nor the precise value of the slope, c_{s1} , is particularly significant. Consequently, c_{s1} will be assigned a value of $2.5 \text{ J kg}^{-1} \text{ K}^{-2}$ for the soils used in this study.

2.5. Advection Associated With Volatilization

[19] Assuming that vaporization of soil moisture acts as a volume source term, the 1-D advective velocity associated with volatilization of water, u_{vl} , has been modeled using a steady state continuity equation [*Ki et al.*, 2005] as

$$\frac{\partial u_{vl}}{\partial z} = -\frac{\rho_w}{(\eta - \theta)\rho_v} \frac{\partial \theta}{\partial t}. \quad (12)$$

Here the basic assumptions are that both liquid water and vapor are Newtonian fluids and that only incompressible effects are being modeled. Although equation (12) is not included in the formal mathematical development of the [*Campbell et al.*, 1995] model, it is briefly discussed in the paper and it is clearly included in the original computer code.

[20] Unfortunately equation (12) proved impossible to use directly in the present model, because the model would not converge (i.e., the solution is nonexistent). Consequently, the present model ensures convergence by a simple multiplicative

adjustment to equation (12), denoted α_u in the following expression:

$$\frac{\partial u_{vl}}{\partial z} = -\alpha_u \frac{\rho_w}{(\eta - \theta)\rho_v} \frac{\partial \theta}{\partial t} \quad (13)$$

where $\alpha_u = 0.5$ was determined by trial and error to always allow convergence. (Note that α_u is reexamined along with issues regarding T_K^* in section 4.2.)

[21] Also note that to ensure that the advective fluxes have the proper sign, i.e., mass and energy are transported toward the free atmosphere above the soil surface, the modeled shear, equations (12) and (13), must satisfy $\partial u_{vl}/\partial z \geq 0$ at all times and depths, which will only occur during evaporation, i.e., when $\partial \theta/\partial t < 0$.

3. Numerical Implementation

[22] The numerical model as outlined above and detailed in this section is coded as MATLAB (The MathWorks Inc., Natick, MA, version R2011b) script files.

3.1. Newton-Raphson Method

[23] The Newton-Raphson method, which is well described by *Campbell* [1985] and *Lynch* [2005], is used to solve the following finite difference forms of equations (9) and (2). Employing the fully implicit (Euler's) finite differencing scheme yields the following heat (H_i) and moisture (W_i) balance functions:

$$H_i = T_i^{j+1} - T_i^j - \rho_w \left(\frac{L_v}{C_s} \right)_i^{j+1} (\theta_i^{j+1} - \theta_i^j) - \frac{\Delta t}{h^2} \left[\left(\frac{\chi_{si+\frac{1}{2}}^{j+1} - \Lambda_{ui}^{j+1}}{C_{si}^{j+1}} \right) T_{i+1}^{j+1} - \left(\frac{\chi_{si-\frac{1}{2}}^{j+1} + \chi_{si+\frac{1}{2}}^{j+1}}{C_{si}^{j+1}} \right) T_i^{j+1} + \left(\frac{\chi_{si-\frac{1}{2}}^{j+1} + \Lambda_{ui}^{j+1}}{C_{si}^{j+1}} \right) T_{i-1}^{j+1} \right] \quad (14)$$

$$W_i = \theta_i^{j+1} - \theta_i^j - \frac{\Delta t}{h^2} \left[\left(\frac{D_{vei+\frac{1}{2}}^{j+1} - \delta_{vi+1}^{j+1}}{\rho_w} \right) \rho_{vi+1}^{j+1} - \left(\frac{D_{vei+\frac{1}{2}}^{j+1} + D_{vei-\frac{1}{2}}^{j+1}}{\rho_w} \right) \rho_{vi}^{j+1} + \left(\frac{D_{vei-\frac{1}{2}}^{j+1} + \delta_{vi-1}^{j+1}}{\rho_w} \right) \rho_{vi-1}^{j+1} \right] \quad (15)$$

where $\delta_{vi}^{j+1} = [0.5h(\eta - \theta)u_{vl}]_i^{j+1}$; $\Lambda_{ui}^{j+1} = [\rho_a c_{pa}]_i^{j+1} \delta_{vi}^{j+1}$; and equations (14) and (15) are second order in the spatial derivatives and center differenced in the gradient-advective terms, δ_{vi}^{j+1} and Λ_{ui}^{j+1} . $\Delta t = 2 \text{ s}$ is the nominal integration time step (although in some model simulations it was decreased in order to ensure numerical stability), $h = 0.001 \text{ m}$ is spatial (vertical) resolution of the model, the superscript j is the time step index, and the subscript i refers to the spatial index with $i = 0$ referring to the surface node and $i = M$ referring to the bottom node. Here the spatial half index $i \pm \frac{1}{2}$ for the soil thermal conductivity and equivalent vapor diffusivity, D_{ve} , refers to the harmonic mean of

their respective values at the i and the $i \pm 1$ nodes, which is in accordance with the flux preserving methods of finite differencing [Lynch, 2005].

[24] Implementing the Newton-Raphson method requires (1) calculating the Jacobian, i.e., the partial derivatives $\partial H_i / \partial T_k$, $\partial H_i / \partial \psi_k$, $\partial W_i / \partial T_k$, and $\partial W_i / \partial \psi_k$ [$\forall k \in \{i-1, i, i+1\}$], and (2) inverting the resulting block-tridiagonal matrix for every time step, Δt , of the simulation. The partial derivatives of the Jacobian are specifically coded in the model as analytical expressions. The block tridiagonal is inverted for each time step with the generalized Thomas algorithm [Karlqvist, 1952; Thomas, 1995; Mendes et al., 2002] and the solution at each time is iterated until the following global energy convergence criterion is met:

$$\frac{h}{\Delta t} \sum_{i=0}^M \sqrt{(C_{si} \Delta T_i)^2 + (\rho_w L_{vi} \Delta \theta_i)^2} \leq 10 \text{ W m}^{-2}$$

where $\Delta \theta_i = \frac{\partial \theta}{\partial \psi} \Delta \psi_i$ and the partial derivative $\frac{\partial \theta}{\partial \psi}$ is determined analytically from the water retention curve, equation (7). Most of the time convergence is usually achieved in three to ten iterations, but can take as many as fifty or more. The tridiagonal form of the solution assumes the application of the upper and lower boundary conditions, which are outlined next.

3.2. Upper Boundary Condition

[25] The upper boundary condition is formulated in terms of the surface energy balance.

$$\epsilon(\theta_0) Q_R^\downarrow(t) = \epsilon(\theta_0) \sigma T_{K0}^4 + \rho_a(T_{K0}) c_{pa} C_H [T_0 - T_a(t)] + L_{v0} E_0 + G_0 \quad (16)$$

where the 0 subscript refers to the surface and the terms from left to right are: the incoming or downwelling radiant energy, $Q_R^\downarrow(t)$ (W m^{-2}), absorbed by the surface, which is partitioned into the four terms (fluxes) on the right side of the equation: the infrared radiation lost by the surface, the surface sensible or convective heat, the surface latent heat, and the surface soil heat flux. $Q_R^\downarrow(t)$ is a function of time and is prescribed as an external condition as discussed a little later. The soil surface emissivity is $\epsilon(\theta_0)$ (dimensionless), which is a function of soil moisture and parameterized as $\epsilon(\theta_0) = 0.93 + 4\theta_0^2(9 - 20\theta_0)/27$ when $0 \leq \theta_0 \leq 0.3$ and $\epsilon(\theta_0) = 0.97$ when $\theta_0 \geq 0.3$. $\sigma = 5.670 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$ is the Stefan-Boltzmann constant.

[26] For the surface sensible heat flux, $\rho_a(T_{K0}) c_{pa} C_H [T_0 - T_a(t)]$, $\rho_a(T_{K0})$ (kg m^{-3}) is the mass density of the ambient air at the surface temperature, T_{K0} (K). Here $\rho_a(T_{K0}) = 1.29(P_a/P_{ST})(T_{ST}/T_{K0})$. C_H (m s^{-1}) is the transfer coefficient for convective heating. For the present model $C_H = 0.032$ (m s^{-1}) is assumed as an approximate average of the wildland fire observations of Butler [2010]. $T_a(t)$ (C) is the ambient temperature somewhere above the soil surface and like incoming radiation is also prescribed externally.

[27] Nonetheless, despite the care taken in the present treatment of the surface convective heat flux, it was still necessary for the laboratory simulations used in the present study to impose the condition that $T_0 - T_a(t) > 0$ C before allowing this term to contribute to the surface energy balance. This is because $T_a(t)$ as a boundary forcing function will always increase faster than T_0 , which might be expected

because as a model response variable T_0 always lags behind $T_a(t)$. That is, in reality for most model simulations developed for the present study, $T_0 - T_a(t) < 0$ C, which then allowed the sensible heat flux to become a significant (and physically implausible) heat source to the soil surface (often resulting in a numerical instability).

[28] The surface evaporation rate, E_0 ($\text{kg m}^{-2} \text{ s}^{-1}$), is parameterized as the sum of a nonadvective (traditional) component and an advective component:

$$E_0 = C_E h_{s0} [\rho_{v0} - \rho_{va}(t)] + C_U u_{v0} \rho_{v0} \quad (17)$$

where C_E (m s^{-1}) and C_U (dimensionless) are adjustable model parameters transfer coefficients, which were determined empirically to maximize E_0 without destabilizing the model. $C_U = 0.25$ is associated with the jet of volatized air emanating from the soil and $C_E = 10^{-3} \text{ m s}^{-1}$. The surface humidity, h_{s0} , is obtained from the Kelvin equation, equation (3). Finally, in the case of the laboratory experiments of Campbell et al. [1995], $\rho_{va}(t)$, along with $T_a(t)$ and $Q_R^\downarrow(t)$, is an external forcing function at the soil surface.

[29] For the unique laboratory conditions of Campbell et al. [1995] these boundary forcing functions take the following generic form:

$$V(t) = V_{in} e^{-t/\tau} + V_f (1 - e^{-t/\tau})$$

where V_{in} is the value of the function at the beginning of the soil heating experiment, V_f is the value of the function at the end of the experiment, and τ (s) is a time constant of the heating source. All these input boundary condition parameter values vary with each individual soil heating experiment. Typical values for $T_a(t)$ are $T_{in} = 22$ C and $T_f = 600$ C, for vapor pressure, $e_{va}(t)$, (from which $\rho_{va}(t)$ is computed by combining with $T_a(t)$ and the ideal gas law) $e_{va,in} = 1000$ Pa and $e_{va,f} = 5000$ Pa, and $1 \text{ s} \leq \tau \leq 600$ s. For the present study all V_f and V_{in} values, except $Q_{Rf}^\downarrow$, are the same as in the original Campbell et al. [1995] model runs. Here $Q_{Rf}^\downarrow$ is adjusted to ensure that the uppermost soil temperature time series are well simulated by the model. This was done in order to compensate for the difference in soil heat capacities between the present study, equation (11), and Campbell et al. [1995], which did not include any temperature dependency. As a consequence, $25,000 \text{ Wm}^{-2} \leq Q_{Rf}^\downarrow \leq 50,000 \text{ Wm}^{-2}$ for all simulations with the present model.

[30] Incorporating the boundary conditions on the balance equations $H_{i=0}$ and $W_{i=0}$ is straightforward and yields the following expressions:

$$H_0 = T_0^{j+1} - T_0^j - \frac{\Delta t}{h^2} \left(\frac{\chi_{s-\frac{1}{2}}^{j+1} + \chi_{s\frac{1}{2}}^{j+1}}{C_{s0}^{j+1}} \right) [T_1^{j+1} - T_0^{j+1}] - \frac{\Delta t}{h^2} 2h \left(1 + \frac{\Lambda_{u0}^{j+1}}{\chi_{s0}^{j+1}} \right) \left(\frac{G}{C_s} \right)_0^{j+1} - \rho_w \left(\frac{L_v}{C_s} \right)_0^{j+1} (\theta_0^{j+1} - \theta_0^j) \quad (18)$$

$$\begin{aligned}
W_0 = & \theta_0^{j+1} - \theta_0^j - \frac{\Delta t}{h^2} \left(\frac{D_{ve-\frac{1}{2}}^{j+1} + D_{ve\frac{1}{2}}^{j+1}}{\rho_w} \right) [\rho_{v1}^{j+1} - \rho_{v0}^{j+1}] \\
& - \frac{\Delta t}{h^2} 2h \left(1 + \frac{\delta_{-1}^{j+1}}{D_{ev0}^{j+1}} \right) \left[\frac{C_E h_{s0}^{j+1} [\rho_{v0}^{j+1} - \rho_a(t)]}{\rho_w} \right] \\
& + \frac{\Delta t}{h^2} \left(\frac{\delta_1^{j+1} - \delta_{-1}^{j+1}}{\rho_w} \right) \rho_{v1}^{j+1} \\
& - \frac{\Delta t}{h^2} \left(1 + \frac{\delta_{-1}^{j+1}}{D_{ev0}^{j+1}} \right) \left(\frac{4\delta_0^{j+1}}{\rho_w} \right) (C_U - 1) \rho_{v0}^{j+1}.
\end{aligned} \tag{19}$$

These expressions for H_0 and W_0 are included here primarily for completeness and it should be noted that (1) the $i = -\frac{1}{2}$ index for the soil thermal conductivity, λ_s , and the equivalent vapor diffusivity, D_{ve} , refer to their respective surface values λ_{s0} and D_{ve0} and (2) $\delta_{-1}^{j+1} \equiv \delta_0^{j+1}$ by the same convention.

3.3. Lower Boundary Condition and Initial Conditions

[31] A numerical lower boundary condition [Thomas, 1995] is used at $i = M$ for the present model. This yields the following relations:

$$T_{M+1}^{j+1} = 2T_M^{j+1} - T_{M-1}^{j+1} \quad \text{and} \quad \psi_{vM+1}^{j+1} = 2\psi_{vM}^{j+1} - \psi_{vM-1}^{j+1}$$

Additionally $\lambda_{sM+\frac{1}{2}} \equiv \lambda_{sM}$ and $D_{veM+\frac{1}{2}} \equiv D_{veM}$. These assigned values of λ_s and D_{ve} at the lower boundary are completely analogous to their counterparts at the upper boundary.

[32] The numerical boundary conditions above are equivalent to the analytical boundary condition $\partial^2 T / \partial z^2 = 0$ and $\partial^2 \psi / \partial z^2 = 0$ at $z = z_M$. They can be thought of as a “pass through” boundary condition, in which the model variables at the lower boundary become part of the numerical solution while the corresponding fluxes are transmitted through the lower boundary. This simplification is used in the present study because specifying the boundary conditions externally from data obtained during a wildfire or a prescribed burn is extraordinarily difficult or impossible to do. Consequently employing these numerical boundary conditions, rather than observationally based analytical boundary conditions, seems a more realistic test of the model.

[33] Nonetheless, the present lower boundary conditions are different than that used by Campbell *et al.* [1995], who used the (time-dependent) soil temperature and moisture measured near the bottom of a heated soil column as an analytical lower boundary condition, i.e., $T_M = T_{\text{measured}}(t)$ and $\theta_M = \theta_{\text{measured}}(t)$. These soil columns were created by packing different (and well-described) soils into cylinders with highly insulated sides. These cylinders were 0.12 m in diameter and 0.155 m deep. For the present 1-D model the modeling domain is 0.20 m deep, which exceeds the depth of the soil column used in the laboratory in order to minimize any influence that the lower boundary condition could have on the model simulations.

[34] The differential equation that describes the advective velocity u_{vb} , equation (12) or equation (13), also requires a lower boundary condition. This is

$$u_{v|M} = 0$$

which is apropos to the physical experiments, as developed and described by Campbell *et al.* [1995], that enclose the heated soil samples in a container with a solid impermeable bottom.

[35] Finally the initial conditions (soil temperature and moisture content), which assumed to be uniform throughout the soil column for each soil type and heating experiment, are taken directly from Campbell *et al.* [1995].

4. Results

4.1. Brief Description of the Experimental Setup

[36] The overall performance of the present model is assessed using the same observed soil temperature and moisture data that Campbell *et al.* [1995] used to evaluate the performance of their soil heating model. As such, all soil temperatures were measured with copper-constantan thermocouples at the sample surface and at 5, 15, 25, 35, 65, and 95 mm depth. Changes in soil moisture were obtained by gamma ray attenuation at the same depths (except the surface). The moisture detecting system was linearly calibrated for each experimental run between (a) the initial soil moisture amounts, which were determined gravimetrically beforehand, and (b) the point at which the sample was oven-dried (also determined before the heating experiment) where $\theta = 0$ is assumed. But oven-drying a soil will not necessarily remove all the liquid water from a soil, i.e., a soil can display residual water content after oven-drying. Consequently, the soil moisture data obtained by Campbell *et al.* [1995] show negative soil moistures at the time the soil dryness passes outside the oven-dry range. Temperature and moisture data were recorded frequently and simultaneously, but at irregular intervals. This is because the gamma ray detection system required several minutes to complete a full profile of the sample. Campbell *et al.* [1995] provide further details concerning the laboratory setup, the gamma ray system, and the data.

[37] In addition to these laboratory experiments, soil heating and moisture data during an experimental slash pile burn [Massman *et al.*, 2008, 2010] are also used to assess the significance of the volatilization-induced advective flow term to soil heating and vapor transport during wildfires and prescribed burns.

4.2. Model Performance

[38] Campbell *et al.* [1995] used several soils with differing initial conditions for their model validation study. But for the present purposes, it is only necessary to report the results for one soil type, i.e., Quincy sand with an initial volumetric soil moisture content of $0.14 \text{ m}^3 \text{ m}^{-3}$.

[39] Figure 2 compares the measured (symbols) and modeled (lines) soil temperature during the Quincy sand heating experiment. The colors indicate the depths (mm) of the experimental and model data. The corresponding measured and modeled soil moisture is shown in Figure 3. Ostensibly, these Figures 2 and 3 indicate that the present model produces results that are similar to both the original Campbell *et al.* [1995] model and the observations [see Campbell *et al.*, 1995, Figures 2C and 3C]. Both models faithfully simulate the hiatus or pause in the soil temperature rise during the evaporative (or drying) period and an increase in soil moisture ahead of the rapidly drying depths

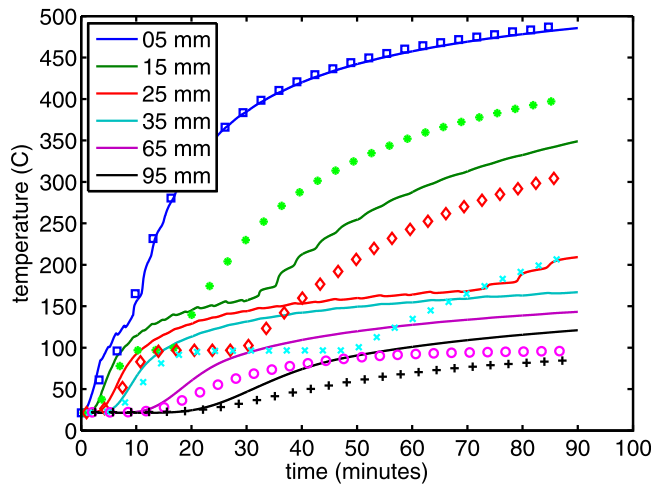


Figure 2. Comparison of measured (symbols) and modeled (lines) soil temperature during the Quincy sand heating experiment. The initial soil moisture content is $0.14 \text{ m}^3 \text{ m}^{-3}$ (see Campbell *et al.* [1995] for further details), and the various depths are color-coded with similar colors.

(presumably due to the transport of evaporated soil moisture to cooler regions deeper in the soil—note: the relative importance of diffusive and advective transport is discussed later in this section). But given the differences between the present model and the original Campbell model, precise agreement between the two model should not be expected. Nonetheless, Figures 2 and 3 (and other model simulations that are not shown here) are quite similar to many of the other model simulations shown by Campbell *et al.* [1995]. But, upon a closer inspection, especially of the soil moisture results, there are some glaring differences between the present model and the observed data, and the original model as well.

[40] These differences are most obviously displayed in the next four figures. Figure 4 shows the observations plotted

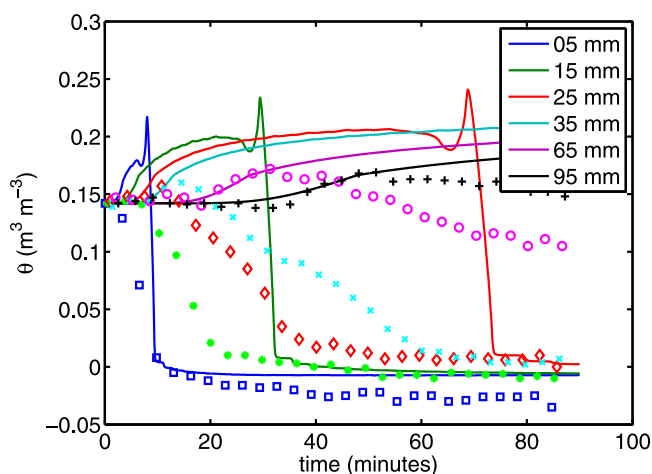


Figure 3. Comparison of measured (symbols) and modeled (lines) soil moisture content during the Quincy sand heating experiment. The initial soil moisture content is $0.14 \text{ m}^3 \text{ m}^{-3}$ (see Campbell *et al.* [1995] for further details), and the various depths are color-coded with similar colors.

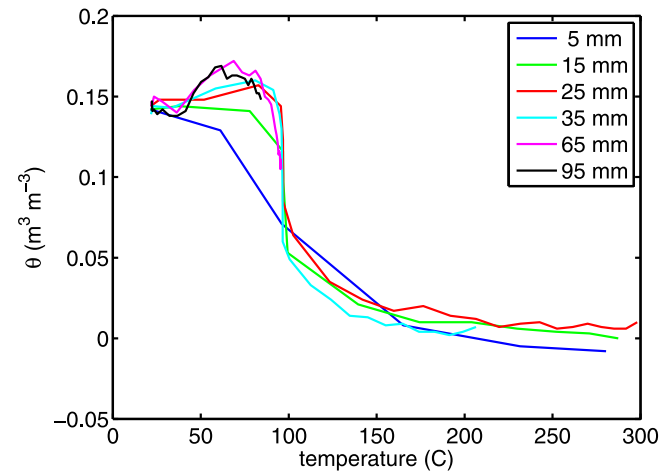


Figure 4. Measured soil moisture versus measured soil temperatures for the Quincy sand heating experiment (see Figures 2 and 3).

as temperature versus soil moisture for all the monitored depths. For the model this type of plot is termed a “solution space” or “ θ - T ” plot, which for the present model simulation is shown in Figure 5. Figure 4 clearly indicates that the temperature at which the soil moisture evaporates most quickly (or the “evaporative front” temperature) is at about 90 C, which of course is also the temperature of the pause in the soil temperature rise. But the model results indicate that the evaporative front occurs at temperatures between about 100 and 180 C and that this evaporative front temperature also increases with the depth. Furthermore, Figure 5 suggests that the amount of evaporated moisture that is recondensing ahead of the evaporative front (i.e., deeper into the soil) is not only much greater than that observed (Figure 4), but that it also is increasing with depth as well. All this suggests that not enough of the modeled evaporated soil moisture is escaping the soil through the upper surface, but rather

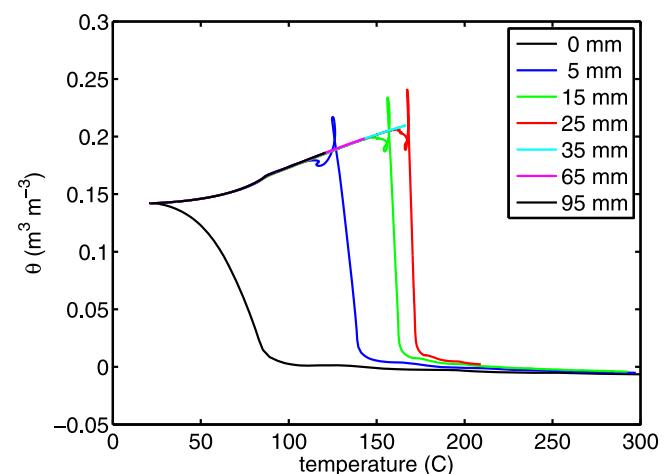


Figure 5. Modeled soil moisture versus measured soil temperatures for the Quincy sand heating experiment (see Figures 2 and 3). This is the solution space representation of the model solution, which is to be compared with the observations shown in Figure 4.

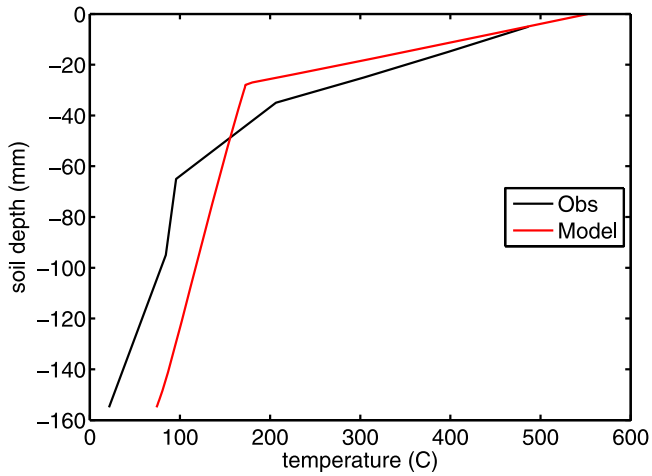


Figure 6. Comparison of the modeled and measured temperature profiles at the completion of the Quincy sand heating experiment. The data shown in the measured profile are not precisely coincident in time (see text for further details).

is being driven deeper into the soil. This is confirmed by Figures 6 and 7.

[41] Figure 6 compares the vertical profiles of the soil temperatures at the end of the laboratory experiment with those at the end of the numerical simulation, and Figure 7 makes a similar comparison for the volumetric soil moisture content. (Note that as was discussed above, the final vertical profiles obtained from the laboratory experiment are approximate only because the final measurements for any given depth are not precisely coincident in time with the measurements made at any other depth. Nevertheless, this is not a significant issue for the present purposes.) The temperature profiles indicate that the model underpredicts

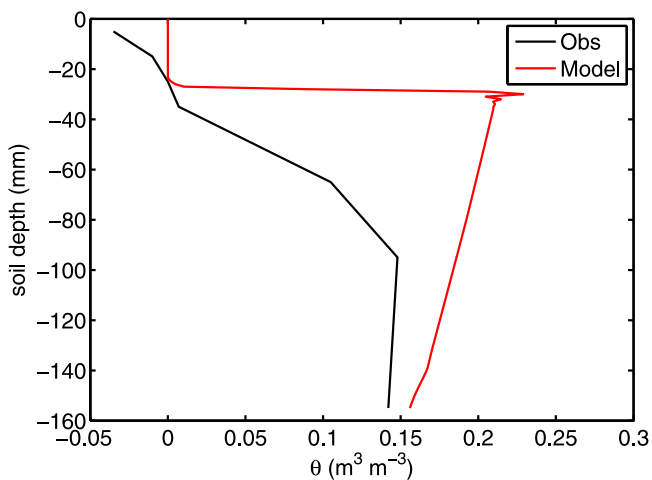


Figure 7. Comparison of the modeled and measured temperature profiles at the completion of the Quincy sand heating experiment. The data shown in the measured profile are not precisely coincident in time (see text for further details). Note the large increase in soil moisture ahead of the drying front (located at about 30 mm depth).

the temperatures in the upper third of the soil column and overpredicts them in the lower two thirds. This is mainly because the soil moisture recondensing ahead of the evaporative front (located at about 30 mm on Figure 7) increases the soil thermal conductivity just ahead of the front so much that the modeled heat being transported (conducted) from the upper part of the soil column to the lower part is much greater than would be expected from the observations.

[42] But an even more surprising result is obtained from comparing the total water lost during the laboratory experiment with that derived from the model simulations. The observed data suggest that about 35% of the original soil moisture has evaporated during the (approximate) 90 min experiment; whereas, virtually none of the original soil moisture has been lost in the model simulations. Rather than actually transporting the evaporated water out of the soil column, the model has “pushed” it deeper into the soil ahead of the evaporative front. This is clearly not something that could have easily been anticipated from the description of the performance of the original model of *Campbell et al.* [1995], who suggested that (at least for Quincy sand and the Boulder creek soil samples) the model produced about a 25% loss. Consequently, this particular measure of model performance suggests that the present model produces a fundamentally different type of solution than the original model. In fact the present solution is somewhat reminiscent of what one might expect if the model had been posed in terms of a Stefan-like or moving boundary condition problem [e.g., *Whitaker and Chou*, 1983–1984; *Liu et al.*, 2005]. Nevertheless, the specific reason for this difference in the solutions produced by the present model and the *Campbell et al.* [1995] model is not clear. But the reason for the present (nonphysical) model solution is clearly displayed in the next figure.

[43] Figure 8 shows the modeled profile of vapor density, $\rho_v(z)$, at the end of the two 90 min model simulations: one with $u_{v,l}$ (leftmost curve) and one without (rightmost curve).

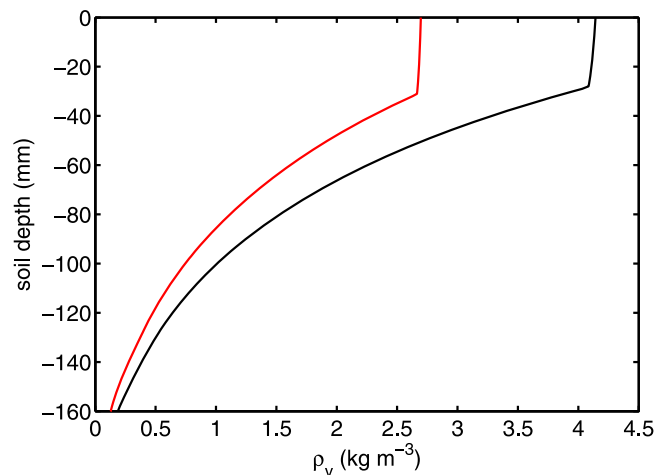


Figure 8. Modeled profiles of the vapor density at the end of the 90 min model simulation. The leftmost curve corresponds to the simulation that includes $u_{v,l}$, equation (13), and the rightmost curve does not include $u_{v,l}$. The vapor density in the dry region (0–30 mm) is physically unrealistic (atmospheric density of air at STP = 1.3 kg m^{-3}) because of the inappropriate use of the Kelvin equation.

According to these model runs, the vapor density is quite high within the extremely hot and dry zone (i.e., the top 30 mm or so) and much lower in the cooler regions deeper in the model domain. In fact the maximum soil vapor density predicted by the model is between about 2.7 and 4.2 kg m⁻³, which is physically unrealistic when one considers that one ambient atmosphere at STP is approximately 1.3 kg m⁻³. Nevertheless, these results do explain the nature of the model solution, which is demonstrated by calculating of the soil humidity, h_s , for a dry soil at several different temperatures.

[44] In order to be consistent with the present model simulations the following calculations assume $\psi = -1.25$ MJ kg⁻¹ for a completely dry soil. For $T_K = 300$ K, 350 K, 650 K, and 850 K this yields: $h_s(300 \text{ K}) = 0.012\%$; $h_s(350 \text{ K}) = 0.044\%$; $h_s(650 \text{ K}) = 1.6\%$; and $h_s(850 \text{ K}) = 4.1\%$. In other words, the soil humidity increases with increasing temperature, i.e., $\partial h_s / \partial T > 0$. Combining this result with $\partial \rho_{sat} / \partial T > 0$ (at least up to the critical temperature of water) yields $\partial \rho_v / \partial T > 0$, $\forall T > 0$ C and $\forall \psi < 0$. So as the temperature rises the dry soil humidity rises, which when coupled with the exponential rise in saturation vapor density, autonomously creates soil vapor far in excess of what is physically realistic.

[45] But u_{vl} also plays an important part in the modeled ρ_v . Through its ability to accelerate moisture loss, u_{vl} produces a final model value of ψ that is slightly greater (-1.09 MJ kg⁻¹) than that produced without it (-1.25 MJ kg⁻¹). Consequently, both h_s and ρ_{v0} are higher at the same temperatures with u_{vl} than without it (i.e., $\partial h_s / \partial \psi < 0$).

[46] Dynamically then, the following picture of the model solution emerges. After an initial burst of the soil surface moisture, E_0 is driven mostly by ρ_{v0} , equation (17) (because $\rho_{va}(t) < 0.013$ kg m⁻³ at all times, so it is always relatively small compared to ρ_{v0}), which in turn increases monotonically with temperature. In the region below the dry front the vapor gradient, $\partial \rho_v / \partial z$, is extremely large and positive so the evaporated soil moisture cannot escape through the soil surface and into the free atmosphere above the soil column, but can only be driven deeper into the soil (or deeper into the modeling domain). Consequently, in the dry zone the evaporative flux is simply removing the autonomously created vapor; while the diffusive flux, which is dominant in the moist zone ahead of the evaporative front transports evaporated soil moisture deeper into the soil.

[47] The model's ability to "push" moisture deeper into the soil ahead of the dry front is also the cause of model instabilities, which occur because as the soil moisture increases $\psi \rightarrow 0$. If soil moisture increases fast enough or becomes large enough, then instead of ψ remaining bounded by zero (i.e., $\psi < 0$) $\psi > 0$ occurs due to a loss of numerical precision. As a result of $\psi > 0$ the corresponding value of θ becomes an imaginary number and the model fails. In fact, the oscillations of the soil moisture near the evaporative front shown in Figure (7) indicates that for the present choice of parameters the model is close to an instability. The original Campbell *et al.* [1995] model also suffers from this same type of instability. On the other hand, this instability issue is alleviated somewhat in the present model by using WRC given by equation (7), which permits θ to be greater for an given ψ , than the original WRC, equation (6). Nonetheless, this instability will always be more likely for any

soil that is relatively moist compared to the same soil with drier initial conditions.

[48] Clearly the roles of the ρ_v and the Kelvin equation are central to the model's failure, but in reality they are merely byproducts of the WRC's (equations (6) and (7)) inability to describe the relationship between soil moisture content and soil water potential for very dry soils (i.e., when $\theta < 0.01$). These low moisture contents are more properly understood as "bound" or "residual" water, rather than "free" water. Therefore, adopting the intuitive notion that ψ_{od} represents the amount of physical work required to oven dry a soil, i.e., vaporize all the free water, then to completely dry out a soil must require greater physical work ($\psi_{\theta=0}$) than ψ_{od} . Or more specifically $|\psi_{\theta=0}| > |\psi_{od}|$ at least, but more likely $|\psi_{\theta=0}| \gg |\psi_{od}|$. Neither equation (6) or (7) is adequate for this situation, implying that this is also an issue with the original Campbell *et al.* [1995] model as well.

[49] On the other hand, if the current WRCs properly allowed for $\psi_{\theta=0}$, then h_s would be significantly reduced, possibly to the point where ρ_v was, not only physically more realistic, but also numerically insignificant. Within limits this hypothesis is testable by evaluating model performance after artificially increasing ψ_{od} (to -4 MJ kg⁻¹), while simultaneously limiting the vapor saturation calculations to $T_K \leq T_K^*$ and increasing α_u , the adjustment parameter associated with the volatilization velocity u_{vl} (equation (13)), to its nominal value of 1. Although the results were encouraging, they were not necessarily conclusive. The limiting or maximum value of ρ_v was much more realistic, i.e., the vapor density at the surface $\rho_v(0) \approx 0.5$ kg m⁻³, and u_{vl} did not have to be artificially reduced. Unfortunately, the model ceased to converge after about 4 min of simulated heating. Nevertheless, the solution at this time was quite similar to that already discussed (Figures 2, 3, 5, 6, and 7). Likewise, the final vertical gradient of ρ_v was just a weaker version of those shown in Figure 8. In summary, model convergence and stability issues involving T_K^* and α_u and the nonphysical nature of the model solution and ρ_v , all appear at least in part to be linked to the structure of the WRC and its inability to capture the evaporative dynamics of bound water.

[50] There can be little doubt that improving modeling of soil heating and moisture transport during fires is likely to require improving understanding of the thermodynamics of bound water and better parameterizations of the WRC. But there are two other aspects of this issue that are worthy of discussion. First, it might be tempting to employ a WRC that allows $\psi_{\theta=0}$ to be unbounded, i.e., $\psi_{\theta=0} = -\infty$. To the author at least, this would seem an unlikely approach for improving model realism because it risks either (1) numerical instabilities as $\theta \rightarrow 0$ (which will be driven by the heating dynamics) because $\psi \rightarrow -\infty$ or (2) another physically unrealistic solution in which the model cannot evaporate all the soil moisture despite heating the soil to several hundred degrees Celsius. Second, a more useful approach to the present modeling dilemma might be to directly incorporate ρ_v as model variable. This has some potential to reduce the problems introduced by the Kelvin equation and the saturation vapor density, both of which are exponential in the other model variables, T_K and ψ , and both of which amplify the weakness of WRC.

4.3. Additional Considerations Regarding u_{vl} and ψ_T

[51] Given the importance of u_{vl} to the performance of the present, and potentially any other, model there are two other aspects of the volatilization-induced advective flow that are worth discussing: first is its intrinsic significance to heat flow (equations (14) and (18)) and to mass flow (equations (15) and (19)), and second is its potential relevance to field application. First, with the present model $\Lambda_u/\lambda_s < 0.01$ during the entire simulation and $\Lambda_u/\lambda_s < 0.003$ during most of the simulation. For vapor flow $\delta_v/D_{ve} \approx 0.2$ during the initial burst of soil surface moisture and otherwise decreasing to $\delta_v/D_{ve} < 0.05$ during most of the rest of the simulation. Consequently, the u_{vl} term can be neglected for heat flow without significantly compromising the model and that all impacts of u_{vl} on soil temperatures occur as a result of its ability to influence evaporation and the resulting soil moisture distribution.

[52] Second, Figure 9 is a θ - T plot for a prescribed slash pile burn performed at Manitou Experimental Forest in April 2004 [Massman *et al.*, 2008, 2010]. These data were obtained every half hour over a 5 day period at an 0.05 m depth under the center of a large slash pile burn. The time series shown in Figure 9 proceeds clockwise from the top left corner, which corresponds to the soil temperature and volumetric moisture at the time the burn was initiated. The rate of change in soil moisture during the evaporative phase in Figure 9 suggests that $\partial\theta/\partial t \approx 0.06 \times 10^{-4} \text{ m}^3 \text{ m}^{-3} \text{ s}^{-1}$. Whereas, Figure 4 and other lab experiments with different soil types suggests that $\partial\theta/\partial t$ varies within $(6 \pm 4) \times 10^{-4} \text{ m}^3 \text{ m}^{-3} \text{ s}^{-1}$ (2 orders of magnitude greater than the field observations). This comparison indicates that u_{vl} is likely to be negligible in field experiments. But these different

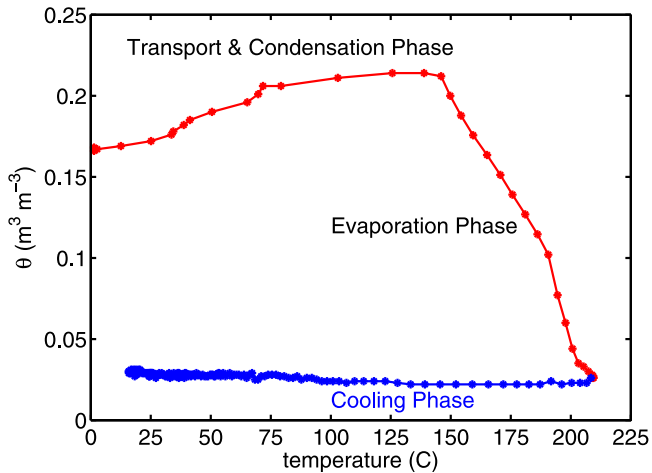


Figure 9. The θ - T (solution space) diagram at 0.05 m depth at the center of a prescribed slash-pile burn performed at Manitou Experimental Forest in April 2004 [Massman *et al.*, 2008, 2010]. The red portion of the curve corresponds to the soil heating phase of the burn, and the blue portion corresponds to the cooling phase. The data points indicated by stars were recorded at half-hourly intervals. The total length of the time series is 5 days (240 half hours), with time proceeding clockwise from the top left corner, which corresponds to the soil temperature and volumetric moisture at the time the burn was initiated.

values of $\partial\theta/\partial t$ only reflect the differences in soil heating that can be achieved in the lab and the field. Unsurprisingly, the rate of forcing during the lab experiments, $\partial Q_R^\downarrow/\partial t|_{t=0} = Q_{Rf}^\downarrow/\tau$, exceeds, by 2–3 orders of magnitude, the soil forcing, $\partial G_0(t)/\partial t$, achieved during the Manitou slash pile burn. (Note that $\partial G_0(t)/\partial t$ is estimated from Figure 3 of Massman *et al.* [2010]). Although $u_{vl} \approx 0$ may be valid in the field, it does not fundamentally alter the present model's performance or nonphysical behavior, which will always produce the same physically unrealistic solution shown in Figure 8.

[53] Finally, it is important to note that ψ_T had very little impact on the present model's performance. Nonetheless, although its influence on moisture dynamics was fairly small at all times, overall it should be characterized as a small improvement to the model.

5. Summary and Recommendations

[54] The present model largely employs standard equations, concepts, and methods for modeling coupled heat and moisture flow in soils, but applies them to the extremes in temperatures and moisture contents that occur during the slash pile burns and wildfires. The model includes temperature dependencies that are not often employed in model formulations of the daily cycles of soil heating and evaporation and advective effects associated with the volume expansion of air that occurs during the rapid volatilization of the soil moisture. Comparing the model simulations with laboratory observations showed that the model produced a numerically stable, but physically unrealistic, solution. The model's shortcomings were traced to the inability of the water retention curve to adequately describe the relationship between soil moisture and soil water potential for very low soil moistures ($\theta < 0.01$, for example). This is a significant result because many present-day WRCs are modeled after the ones used in this study, suggesting that even under less extreme heating conditions many (if not most or all) present-day models of soil evaporation will fail at extremely low soil moistures.

[55] Although the weakness of the present model may limit its utility, it does offer insights into how to design a more physically realistic model. First, improved understanding and models of the thermodynamics of evaporation of bound water are a clear necessity. Field data shown in Figure 9, as well as the lab data shown in Figure 4, and all the other laboratory results shown in Campbell *et al.* [1995] that are not included in the present study, clearly indicate that soil moisture is retained in the soil until the soil has been heated to between 200 C and somewhere above 300 C (well above the temperature for oven drying a soil). These data obviously support the need for improving WRCs near the dry end and beyond the oven-dried state. Second, a dual-phase model, one in which θ and ρ_v are modeled separately, is likely to be required. Such a model could employ either an "equilibrium" or a "nonequilibrium" evaporation approach [e.g., Smits *et al.*, 2011], which in either case would reduce the role that the Kelvin Equation and the saturation vapor density play in the numerical calculations of the present model. Third and final, it may be beneficial to include hydraulic conductivity in the model to permit liquid water movement in response to the

extremely high moisture potential gradients that invariably occur during fires.

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